

ADVANCED SIMULATION OUTPUT ANALYSIS FOR A SINGLE SYSTEM

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ABSTRACT

This paper reviews advanced statistical methods for analyzing output data from computer simulations of single systems. In particular, it focuses on the problems of choosing initial conditions and estimation of steady-state system parameters. The estimation techniques include the replication/deletion approach, the regenerative method, variations of the batch means method, the autoregressive method, the spectral estimation method, and the standardized time series method.

1 INTRODUCTION

The primary purpose of most simulation studies is the approximation of certain system parameters with the objective of identifying parameter values that optimize some system performance measures. If some of the input processes driving a simulation are random, then the output data are also random and runs of the simulation program only give *estimates* of system performance characteristics. Unfortunately, a simulation run does not usually produce i.i.d. observations; therefore "classical" statistical techniques are not directly applicable to the analysis of simulation output.

A simulation study consists of several steps such as data collection, coding and verification, model validation, experimental design, output data analysis, and implementation. This paper focuses on the use of output data for estimating system performance measures.

There are two types of simulations with regard to output analysis:

1. *Terminating (or transient) simulations.* The termination of a transient simulation is caused by the occurrence of an event E . An example is the simulation of a production system until a given machine breaks down.

2. *Nonterminating (or steady-state) simulations.* The purpose of a steady-state simulation is the study of the long-run behavior of the system of interest. A performance measure of a system is called a *steady-state parameter* if it is a characteristic of the equilibrium distribution of an output stochastic process (Law and Kelton 1991). An example is the simulation of a continuously operating communication system where the objective is the computation of the mean delay of a data packet.

Section 2 discusses methods for analyzing output from terminating simulations. Section 3 reviews approaches for removing bias due to initial conditions in steady-state simulations. Section 4 presents techniques for point and interval estimation of steady-state parameters. Finally, section 5 contains conclusions and recommendations for additional studies by the interested reader.

2 TERMINATING SIMULATIONS

We start with the output analysis methodology for terminating simulations. Suppose that we simulate a system until m output data X_1, X_2, \dots, X_m are collected with the objective of estimating $\mu = E(\bar{X}_m)$, where $\bar{X}_m = \frac{1}{m} \sum_{i=1}^m X_i$ is the sample mean of the data. For example, X_i may be the transit time of unit i through a network of queues or the total time station i is busy during the i th hour. Clearly, \bar{X}_m is an unbiased estimator for μ . Unfortunately, the X_i 's are generally dependent random variables making the estimation of the variance $\text{Var}(\bar{X}_m)$ a non-trivial problem. In many queueing systems the X_i 's are positively correlated making the familiar estimator $S^2(m)/m = \sum_{i=1}^m (X_i - \bar{X}_m)^2 / [m(m-1)]$ a highly biased estimator of $\text{Var}(\bar{X}_m)$.

To overcome this problem, one can run n independent replications of the system simulation.

Assume that run i produces the output data $X_{i1}, X_{i2}, \dots, X_{im}$. Then the sample means

$$Y_i = \frac{1}{m} \sum_{j=1}^m X_{ij}$$

are i.i.d. random variables,

$$\bar{Y}_n = \frac{1}{n} \sum_{i=1}^n Y_i$$

is also an unbiased estimator of μ , and

$$\hat{V}_R = \frac{1}{n-1} \sum_{i=1}^n (Y_i - \bar{Y}_n)^2$$

is an unbiased estimator of $\text{Var}(\bar{X}_m)$. If in addition m is sufficiently large, an approximate $100(1-\alpha)$ percent two-sided confidence interval for θ is

$$\mu \in \bar{Y}_n \pm t_{n-1, 1-\alpha/2} \sqrt{\hat{V}_R/n}, \quad (1)$$

where $t_{d,\gamma}$ represents the γ -quantile of the t distribution with d degrees of freedom.

Law and Kelton (1991) review sequential procedures for determining the number of replications required to estimate μ with a fixed error or precision. Their procedure for obtaining an estimate with a relative error $|\bar{X}_m - \mu|/|\mu| \leq \gamma$ and a $100(1-\alpha)$ percent confidence interval has performed well for initial sample size $n_0 \geq 10$ and $\gamma \leq 0.15$. A well-known sequential procedure for constructing a $100(1-\alpha)$ percent confidence interval for μ with a small absolute error $|\bar{X}_m - \mu| \leq \beta$ is due to Chow and Robbins (1965) (see also Nadas 1969). Law (1980) observed that the procedure is very sensitive to the value of β .

The method of replications can also be used for estimating performance measures other than means. For example, suppose that we want to estimate the p -quantile, say y_p , of the maximum queue size in a single-server queueing system during a fixed time window. We run n independent replications, denote by Y_i the maximum observed queue length during replication i , and let $Y_{(1)}, Y_{(2)}, \dots, Y_{(n)}$ be the order statistics corresponding to the Y_i 's. Then a point estimate for y_p is

$$\hat{y}_p = \begin{cases} Y_{(np)} & \text{if } np \text{ is an integer} \\ Y_{(\lfloor np+1 \rfloor)} & \text{otherwise} \end{cases}$$

and a confidence interval for y_p is described in Welch (1983, pp. 287-288).

3 INITIALIZATION PROBLEMS FOR STEADY-STATE SIMULATIONS

One of the hardest problems in steady-state simulations is the removal of the *initialization bias*. Suppose that X_1, X_2, \dots is a discrete-time output stochastic process from a single run of a steady-state simulation with initial conditions I and assume that, as $m \rightarrow \infty$, $P(X_m \leq x|I) \rightarrow P(X \leq x)$, where X is the corresponding steady-state random variable. We consider the estimation of the steady-state mean $\mu = \lim_{m \rightarrow \infty} E(X_m|I)$. The problem with the use of the estimator \bar{X}_m for a finite m is that $E(X_m|I) \neq \mu$.

The most commonly used method for eliminating the bias of \bar{X}_m identifies a index $1 \leq l \leq m-1$ and *truncates* the observations X_1, \dots, X_l . Then the estimator

$$\bar{X}_{m,l} = \frac{1}{m-l} \sum_{i=l+1}^m X_i$$

is generally less biased than \bar{X}_m because the initial conditions primarily affect data at the beginning of a run. Several procedures have been proposed for the detection of a cutoff index l (see Fishman 1972; Gafarian, Ancker, and Morisaku 1978; Kelton and Law 1983; Schruben 1982; Schruben, Singh, and Tierney 1983; Wilson and Pritsker 1978a,b). Unfortunately, these procedures do not appear to work well in practice. The procedure of Kelton (1989) uses a *pilot* run to estimate the steady-state distribution and starts a production run by sampling from the estimated distribution. A more sophisticated truncation rule has recently been proposed by Chance and Schruben (1992).

We now briefly discuss the graphical procedure of Welch (1981, 1983) which is simple and general. Another graphical method has been proposed by Fishman (1978a,b) in conjunction with the batch means method (see section 4.3). Welch's method uses n independent replications with the i th replication producing observations $X_{i1}, X_{i2}, \dots, X_{im}$ and computes the averages

$$\bar{X}_j = \frac{1}{n} \sum_{i=1}^n X_{ij} \quad j = 1, \dots, m.$$

Then for a given *time window* w , the procedure plots the moving averages

$$\bar{X}_j(w) = \begin{cases} \frac{1}{2w+1} \sum_{k=-w}^w \bar{X}_{j+k} & w+1 \leq j \leq m-w \\ \frac{1}{2j-1} \sum_{k=-j+1}^{j-1} \bar{X}_{j+k} & 1 \leq j \leq w \end{cases}$$

against j . If the plot is reasonably smooth, then l is chosen to be the value of j beyond which the sequence of moving averages converges. Otherwise, a different

time window is chosen and a new plot is drawn. The choice of w is similar to the choice of an interval width for a histogram.

4 STEADY-STATE ANALYSIS

Several methods have been developed for the estimation of steady-state system parameters. Below we briefly review these methods and provide the interested reader with an extensive list of references. We focus on the estimation of the steady-state mean μ of a (discrete-time) output process $\{X_i, i \geq 0\}$. Analogous methods for analyzing continuous-time output data are described in a variety of texts (Bratley, Fox, and Schrage 1987; Fishman 1978b; Law and Kelton 1991). The process $\{X_i\}$ is called *strictly stationary* if the joint distribution of $X_{i+j_1}, X_{i+j_2}, \dots, X_{i+j_k}$ is independent of i for all indices j_1, j_2, \dots, j_k . If $E(X_i) = \mu$ and $\text{Var}(X_i) = \sigma^2 < \infty$ for all i , and the $\text{Cov}(X_i, X_{i+j})$ is independent of i , then $\{X_i\}$ is called *covariance-stationary*.

4.1 The Replication/Deletion Approach

This approach runs n independent replications each of length m observations and uses the method of Welch (18981, 1983) to discard the first l observations from each run. One then uses the i.i.d. sample means

$$Y_i = \frac{1}{m-l} \sum_{j=l+1}^m X_{ij}$$

to compute point and interval estimators for the steady-state mean μ (see section 2). The method works well if m is sufficiently large and is characterized by its simplicity and generality.

4.2 The Regenerative Method

This method assumes the identification of time indices at which the process $\{X_i\}$ probabilistically *starts over* and uses these regeneration epochs for obtaining i.i.d. random variables which can be used for computing point and interval estimates for the mean μ . The method was proposed by Crane and Iglehart (1974a, 1974b, 1975) and Fishman (1973, 1974). A complete treatment of the regenerative method is given in Crane and Lemoine (1977). More precisely, assume that there are (random) time indices $1 \leq T_1 < T_2 < \dots$ such that the portion $\{X_{T_i+j}, j \geq 0\}$ has the same distribution for each i and is independent of the portion prior to time T_i . The portion of the process between two successive regeneration epochs is called a *cycle*. Let $Y_i = \sum_{j=T_i}^{T_{i+1}} X_j$ and $Z_i = T_{i+1} - T_i$

for $i = 1, 2, \dots$ and assume that $E(Z_i) < \infty$. Then the mean μ is given by

$$\mu = \frac{E(Y_1)}{E(Z_1)}.$$

Now suppose that one simulates the process $\{X_i\}$ over n cycles and collects the observations Y_1, \dots, Y_n and Z_1, \dots, Z_n . Then

$$\hat{\mu} = \frac{\bar{Y}_n}{\bar{Z}_n}$$

is a strongly consistent, although typically biased for finite n , estimator of μ . Furthermore, confidence intervals for μ can be constructed by using the random variables $Y_i - \mu Z_i, i = 1, \dots, n$ and the central limit theorem (see Iglehart 1975). For small sample sizes and bounded Y_i and Z_i , one can compute the confidence interval in Alexopoulos (1993) which provide superior coverage over confidence intervals based on the central limit theorem at the expense of increased width.

The regenerative method is difficult to apply in practice because the majority of simulations have either no regenerative points or very long cycle lengths. A class of systems the regenerative method has successfully been applied to are inventory systems.

4.3 The Batch Means Method

The method of batch means is frequently used to estimate the steady-state mean μ or the $\text{Var}(\bar{X}_m)$. Basic references on the method are Conway (1963), Fishman (1978a,b), Law and Carson (1979), and Schmeiser (1982). The method divides the output X_1, \dots, X_m of a long simulation run into a number of contiguous *batches* and uses the sample means of these batches (or *batch means*) to produce point and interval estimators.

Specifically, we assume that the process $\{X_i\}$ is covariance-stationary with $\text{Cov}(X_i, X_{i+j}) = C_j$ and split the data into n batches, each consisting of k observations (assume $m = nk$). The i th batch consists of the observations

$$X_{(i-1)k+1}, Y_{(i-1)k+2}, \dots, X_{ik}$$

for $i = 1, 2, \dots, n$ and the i th batch mean is given by

$$Y_i(k) = \frac{1}{k} \sum_{j=1}^k X_{(i-1)k+j}.$$

Since the process is covariance-stationary, it can be shown that

$$\begin{aligned} C_i(k) &\equiv \text{Cov}[Y_i(k), Y_{i+l}(k)] \\ &= \frac{1}{k} \sum_{j=1}^{k-1} \left(1 - \frac{|j|}{k}\right) C_{lk+j} \end{aligned}$$

independently of i . Therefore, if the autocovariance function $\{C_j\}$ is such that $C_i(k) \rightarrow 0$ as k increases, we can identify a batch size k for which the batch means $Y_i(k)$, $i = 1, \dots, n$ are approximately i.i.d. normally distributed. Then we form the grand batch mean

$$\bar{Y}_n = \bar{X}_m = \frac{1}{n} \sum_{i=1}^n Y_i(k),$$

estimate the $\text{Var}[Y_i(k)]$ by

$$\hat{V}_B = \frac{1}{n-1} \sum_{i=1}^n (Y_i(k) - \bar{Y}_n)^2,$$

and compute the approximate $100(1-\alpha)$ percent confidence interval for μ

$$\mu \in \bar{Y}_n \pm t_{n-1, 1-\alpha/2} \sqrt{\hat{V}_B/n}.$$

The main problem with the application of the batch means method in practice is the choice of the batch size k . If k is small, the means $Y_i(k)$ will be correlated and the resulting confidence interval will frequently have coverage below the user-specified nominal coverage. Alternatively, a large batch size will likely result in very few observations and potential problems with the applicability of the central limit theorem. An extensive study of batch size effects was conducted by Schmeiser (1982).

A number of procedures have been proposed for determining an appropriate batch size (see Law and Carson 1979; Fishman 1978a,b). Below, we briefly discuss the method of Fishman because of its simplicity and applicability to other analyses as the computation of point and confidence intervals for $m\text{Var}(\bar{X}_m)$, the elimination of initialization bias, and the determination of a sample size m for which $P(|\bar{X}_m - \mu| \leq d) \approx 1$. The interested reader should study the revised notes for chapter 5 of Fishman (1978b) which are available by the author on request.

The method starts with a sample size that is a power of 2 and batches of size 1. Then it goes through a procedure which performs a hypothesis test for lack of autocorrelation between adjacent batch means and successively doubles the batch size (and halves the number of batches) until either no significant amount of autocorrelation is detected or the number of batches is less than 8. In the former case the current batch size is selected while in the latter case additional observations are collected and the procedure is repeated. Schmeiser (1982) observed that if the autocovariance function $\{C_j\}$ is positive and decreasing, then one rarely needs more than roughly 30 batches. Fishman's procedure detects the presence of cyclic behavior in $\{C_j\}$ by computing the p -values

of the hypothesis test for *all* batch sizes k for which $n = m/k \geq 8$. An increasing sequence of p -values is indicative of a monotonically decreasing autocovariance function. We should point out that a plot of the batch means is a very useful tool for checking the effects of initial conditions, nonnormality of batch means, and existence of correlation between batch means.

An interesting variation of the traditional batch means method is the method of *overlapping* batch means proposed by Meketon and Schmeiser (1984). For given batch size k , this method uses all $m-k+1$ overlapping batches to estimate μ and $\text{Var}(\bar{X}_m)$. The first batch consists of observations X_1, \dots, X_k , the second batch consists of X_2, \dots, X_{k+1} , etc. Welch (1987) noted that both traditional batch means and overlapping batch means are special cases of spectral estimation (see section 4.5) at frequency 0 and, more importantly, suggested that overlapping batch means yield optimal variance reduction when one forms sub-batches within each batch and applies the method to the sub-batches. For example, a batch of size 64 is split into 4 sub-batches and the first (overlapping) batch consists of observations X_1, \dots, X_{64} , the second consists of observations X_{17}, \dots, X_{80} , etc.

4.4 The Autoregressive Method

This method was developed by Fishman (1978b) and assumes that the output process $\{X_i\}$ is covariance-stationary with mean μ and $\sum_{j=-\infty}^{\infty} |C_j| < \infty$, and can be represented by the autoregressive model of order p

$$\sum_{j=0}^p b_j (X_{i-j} - \mu) = \epsilon_i,$$

where $b_0 = 1$ and $\{\epsilon_i\}$ is a sequence of uncorrelated random variables with mean 0 and variance σ_ϵ^2 . The procedure in Fishman (1978b) determines an order p and computes estimates \hat{b}_j and $\hat{\sigma}_\epsilon^2$ of b_j and σ_ϵ^2 respectively. Then for large m an approximate $100(1-\alpha)$ percent confidence interval for μ is

$$\mu \in \bar{X}_m \pm t_{d, 1-\alpha/2} \sqrt{\hat{V}_A/m},$$

where

$$\hat{V}_A = \frac{\hat{\sigma}_\epsilon^2}{m \left(\sum_{j=0}^p \hat{b}_j \right)^2}$$

and the degrees of freedom are computed from

$$d = \frac{m \sum_{j=0}^p \hat{b}_j}{2 \sum_{j=0}^p (p-2j) \hat{b}_j}.$$

The major difficulty with the use of the autoregressive method is the validity of the autoregressive model. A generalization of the method was proposed by Schriber and Andrews (1984).

4.5 The Spectral Estimation Method

This method also assumes that the process $\{X_i\}$ is covariance-stationary. Under this assumption, the variance of \bar{X}_m is given by

$$\text{Var}(\bar{X}_m) = \frac{1}{m} \left(C_0 + 2 \sum_{j=1}^{m-1} (1 - j/m) C_j \right).$$

The name of the method is due to the fact that if $\sum_{j=-\infty}^{\infty} |C_j| < \infty$, then $m\text{Var}(\bar{X}_m) \rightarrow 2\pi g(0)$ as $m \rightarrow \infty$, where $g(\lambda)$ is the *spectrum* of the process at frequency λ and is defined by

$$g(\lambda) = \frac{1}{2\pi} \sum_{j=-\infty}^{\infty} C_j e^{-i\lambda j} \quad |\lambda| \leq \pi,$$

where $i = \sqrt{-1}$. Therefore, for large m the estimation of $\text{Var}(\bar{X}_m)$ can be viewed as that of estimating $g(0)$. Estimators of this variance have the form

$$\hat{V}_S = \frac{1}{m} \left(\hat{C}_0 + 2 \sum_{j=1}^{p-1} w_j \hat{C}_j \right),$$

where p and the *weights* are chosen for improving the properties of the variance estimator \hat{V}_S . The selection of these parameters is discussed in Fishman (1978b) and Law and Kelton (1984). Further discussions of spectral methods are given in Heidelberger and Welch (1981a,b, 1983).

4.6 The Standardized Time Series Method

This method was proposed by Schruben (1983). It assumes that the process $\{X_i\}$ is strictly stationary and *phi-mixing* (see Billingsley 1968, p. 166). Informally, $\{X_i\}$ is phi-mixing if X_i and X_{i+j} are approximately independent for large j . Suppose that the data X_1, \dots, X_m are divided into n (contiguous) batches, each of size k , and let $Y_1(k), \dots, Y_n(k)$ be the respective batch means. Then for sufficiently large m the random variables

$$A_i = \sum_{j=1}^k [(m+1)/2 - j] X_{(i-1)k+j} \quad i = 1, \dots, n$$

become approximately i.i.d. normal and an (approximate) $100(1 - \alpha)$ percent confidence interval for μ is

$$\mu \in \bar{Y}_n \pm t_{n,1-\alpha/2} \sqrt{\hat{V}_T/m},$$

where

$$\hat{V}_T = \frac{12}{(k^3 - k)n} \sum_{i=1}^n A_i^2.$$

The standardized time series method is easy to implement and has asymptotic advantages over the batch means method (see Goldsman and Schruben 1984). However, in practice it can require prohibitively long runs as noted by Sargent, Kang, and Goldsman (1992). The theoretical foundations of the method are given in Glynn and Iglehart (1990). Additional developments on the method are contained in Goldsman, Meketon, and Schruben (1990) and Goldsman and Schruben (1984, 1990).

4.7 Quantile Estimation

A variety of methods have been proposed for estimating quantiles of steady-state data (see Iglehart 1976; Moore 1980; Seila 1982a,b; Heidelberger and Lewis 1984). The methods differ in the way the variance of the sample quantile is estimated. It should be mentioned that quantile estimation is a harder problem than the estimation of steady-state means.

4.8 Multivariate Estimation

Frequently, the output from a single simulation run is used for estimating several system parameters. The estimators of these parameters are typically correlated. As an example, consider the average customer delays at two stations on a path of a queueing network. In general, Bonferroni's inequality can be used for computing a conservative confidence coefficient for a set of confidence intervals. Indeed, suppose that D_i is a $100(1 - \alpha)$ percent confidence interval for the parameter μ_i , $i = 1, \dots, k$. Then

$$P(\cap_{i=1}^k \{\mu_i \in D_i\}) \geq 1 - \sum_{i=1}^k \alpha_i.$$

This result can have serious implications as for $k = 10$ and $\alpha_i = 0.10$ the r.h.s. of the above inequality is equal to 0. If the overall confidence level must be at least $100(1 - \alpha)$ percent, then the α_i 's can be chosen so that $\sum_{i=1}^k \alpha_i = \alpha$. The existing multivariate estimation methods include Charnes (1989, 1990, 1991), Chen and Seila (1987), and Seila (1984).

5 CONCLUSIONS

The purpose of this paper is to alert the user on a variety of issues and methodologies related to the analysis of output data from a simulation of a single system. Several aspects of output analysis were left out such

as comparison of systems, design of simulation experiments, and variance reduction methods. These subjects are treated in a variety of articles in this volume, additional publications listed below, and several texts including Bratley, Fox, and Schrage (1987), Fishman (1978b), and Law and Kelton (1991).

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